

NLTE analysis of spectra: OBA stars

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Abstract Methods of calculation of NLTE model atmosphere are discussed. The NLTE trace element procedure is compared with the full NLTE model atmosphere calculation. Differences between LTE and NLTE atmosphere modeling are evaluated. The ways of model atom construction are discussed. Finally, modelling of expanding atmospheres of hot stars with winds is briefly reviewed.

1 Introduction

As hot stars we usually consider stars of spectral types A, B, and O. These stars are hotter than about 8500 K (this temperature value depends on who is classifying them), they are also more massive and have several times larger radius than the Sun. Their spectra may be characterized by fewer spectral lines than cool stars, and by the absence of molecular lines, which is given by their higher temperature. Also thanks to temperature the major convection zone caused by hydrogen ionization is absent in their atmospheres. In addition, strong NLTE effects appear in their atmospheres, which influence not only line formation, but the whole atmospheric structure.

However, they also differ depending on their spectral type. The atmospheres of A-type stars are usually very quiet with almost a total absence of atmospheric motions. Consequently, specific phenomena like chemical stratification of their atmospheres may develop. This is also the reason for strong chemical peculiarities found

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in many of them. The atmospheres of B-type stars are less quiet, and macroscopic atmospheric motions start to appear there. These stars are very often rapidly rotating, which causes development of circumstellar envelopes and emission lines in their spectra (the case of Be stars). On the other hand, many stars of this type are pulsating (e.g. the β Cep type stars), some even show non-radial pulsations. The O-type stars are typified by strong stellar winds, which cause specific emission lines (with P-Cygni type profiles) in their spectra. For all these spectral types, NLTE effects are essential for both atmospheric structure and line formation.

Consequently, the NLTE approach for analysis of their spectra is inevitable. There are two basic possibilities to calculate stellar atmosphere models with the departures from LTE. The first and consistent one is calculation of full NLTE model atmospheres including all chemical elements. However, this option is still computationally prohibitive, so we usually restrict the number of chemical elements and include only those, which are important for the determination of the atmospheric structure. The second option is to solve the NLTE line formation problem for a particular atom or ion (called a trace element) for a given (i.e. fixed) model atmosphere. This model may be calculated assuming either LTE or NLTE. The former option saves significant amount of time necessary for calculations. On the other hand, LTE model atmospheres are physically inconsistent (Mihalas, 1978; Hubeny and Mihalas, 2014).

2 Trace elements

Solution of a NLTE line formation problem for trace elements splits the solution of the problem in two steps.

The first step is a calculation of the model atmosphere, which includes only those elements and their transitions, which are important for determination of the atmospheric structure, specifically continua of abundant elements and strong atomic lines. Many weaker lines in the optical region may be omitted in this step, since their influence on the atmospheric structure is negligible. This model atmosphere may assume either LTE or NLTE, however, a NLTE model atmosphere should be in principle always preferred in this step.

Having a model atmosphere we solve a NLTE line formation problem, i.e. simultaneous solution of the radiative transfer equation and the equations of statistical equilibrium for a selected element (the *trace element*). Since the model atmosphere (i.e. the full structure) is not solved in this step, the model atom may be very detailed and include many lines and continua important for formation of lines of this elements.

Several conditions have to be fulfilled to allow us to consider a particular element as a trace element. First of all, its influence on the atmospheric structure has to be negligible. Also the opacity of the trace element has to be negligible compared to the opacity of non-trace elements, or NLTE effects on opacities of this element have negligible influence on the atmospheric structure. Trace element also should

not be a significant source of free electrons. Simply stated, any detailed trace element calculation *must not* influence the other elements. If this happens, we have to improve the background model. An example of a trace element may be, e.g., argon in B-type stars (Lanz et al, 2008). These authors used fully blanketed NLTE model atmospheres as background models, which is the best available option. More discussion about NLTE for trace elements can be found in Monier et al (2010).

3 Full NLTE model atmospheres

Calculation of a full NLTE model atmosphere is a task, which from basic global stellar parameters like effective temperature (or luminosity), mass, and radius determines spatial distribution of temperature, density, ionization states, electron density, velocity, etc.

We would like to emphasize that the resulting model atmospheres may differ significantly from the LTE solution, as has already been clearly shown by Auer and Mihalas (1969a).

3.1 Solution of a NLTE model atmosphere

Solution of a NLTE model atmosphere means determination of distributions of macroscopic quantities in the stellar atmosphere for given global parameters describing stellar luminosity L_* , mass M_* , and radius R_* . It is achieved via a solution of a system of equations describing physical properties of the atmosphere. We demonstrate these equations for a specific case of the static plane-parallel NLTE model atmosphere. These equations include the equation of radiative transfer, which determines the radiation field described using its specific intensity $I_{\mu\nu}$,

$$\mu \frac{dI_{\mu\nu}}{dz} = \eta_\nu - \chi_\nu I_{\mu\nu}, \quad (1)$$

the equations of statistical equilibrium determining atomic level populations n_i ,

$$n_i \sum_l (R_{il} + C_{il}) + \sum_l n_l (R_{li} + C_{li}) = 0, \quad (2)$$

the equation of hydrostatic equilibrium which determines the density structure ρ ,

$$\frac{dp}{dm} = g - \frac{4\pi}{c} \int_0^\infty \frac{\chi_\nu}{\rho} H_\nu d\nu, \quad (3)$$

and the equation of radiative equilibrium, which determines the temperature structure T ,

$$4\pi \int_0^\infty (\chi_\nu J_\nu - \eta_\nu) d\nu = 0. \quad (4)$$

In these equations, $n_i R_{il}$ and $n_i C_{il}$ are radiative and collisional rates for transitions from level i to level l , respectively, p is the gas pressure, g is gravitational acceleration, c is the light speed, m is the column mass depth ($dm = -\rho dz$), ρ is the density, H_ν is the radiative Eddington flux, J_ν is the mean radiation intensity, η_ν and χ_ν are emissivity and opacity, respectively, and $\mu = \cos \theta$ is an angle cosine of a light ray.

This set of equations has to be solved simultaneously. An efficient method was introduced by Auer and Mihalas (1969b) as the complete linearization method, which is the multidimensional Newton-Raphson Method. If this method is combined with the accelerated lambda iteration method, significant saving of computing time may be achieved (e.g. Hubeny and Lanz, 1992, 1995; Kubát, 1994, 1996, 2003).

3.2 Model atmosphere grids

Since calculation of NLTE model atmospheres is a very time consuming task even for the relatively simple static 1-D case, for practical purposes it is efficient to use precalculated grids of model atmospheres and to interpolate between them if a model for required parameters is not available in the grid.

An example of such a grid is the grid of NLTE model line blanketed atmospheres of O and B stars (Lanz and Hubeny, 2003, 2007). There is also a grid of LTE line blanketed model atmospheres, which covers almost all reasonable temperatures and gravities, consequently also hot stars (Kurucz, 1993).

Using a grid instead of a calculation of a model atmosphere we limit ourselves to several fixed values of grid parameters, which can be for example the stellar effective temperature T_{eff} , gravitational acceleration at the stellar surface g , stellar radius R_* , stellar mass M_* , stellar luminosity L_* , and elemental abundances. Since the parameter space can be quite extended, using a grid calculated for a limited range of parameters for model atmosphere analysis may fail, especially if we want to investigate stars with parameters beyond the grid ones. The most efficient possibility is first to use models from a grid to determine rough values of stellar parameters, which may be then refined using detailed model atmosphere calculations. However, if the model grids have sufficiently dense spacing in basic structural parameters, interpolation of the models may work well, as it was shown by Lanz and Hubeny (2003).

4 Comparison of LTE and NLTE modelling

Since first NLTE model atmospheres were calculated in late 60s (Auer and Mihalas, 1969a), there has always been a discussion if NLTE model atmospheres are really necessary or if LTE models are sufficient. In any case, the NLTE approximation is

more general than the LTE one. The NLTE effects can be quite complicated. Consequently, we can only prove that LTE offers acceptable results *after* we calculate a NLTE model, which is able to verify necessary conditions for LTE. Assuming LTE means assuming detailed balance in *all* transition a priori. Even if we succeed to fit a part of the spectrum with the LTE model atmosphere, it can not be a proof that the LTE model describes the atmosphere well.

The basic advantage of LTE models is the fact that they can be calculated very quickly. Using contemporary computers we can obtain an LTE model within one minute or even faster. On the other hand, calculation of a NLTE model atmosphere may last several hours or even more. A question may arise, if we gain anything from these additional hours of computing time. Of course, we get a lot. NLTE model atmosphere calculations give us more accurate level populations, more accurate ionization balance, more accurate opacities, more accurate radiation field, and more accurate temperature and density structure in resulting models.

Although it is clear that the NLTE model atmospheres are superior to the LTE ones, the latter ones dominated the analysis of hot stars for many years. The reason was the problem of line blanketing, where a huge number of spectral lines in the ultraviolet region caused absorption of radiation, which was the reemitted in the optical region. In LTE, relatively straightforward approximations of opacity distribution function or opacity sampling enabled to handle this effect. On the other hand, in NLTE model atmospheres the influence of the radiation field on level populations had to be taken into account, which was computationally prohibitive until an efficient method enabling treatment of line blanketing in NLTE was developed. This method uses the concept of superlevels and superlines (Anderson, 1989). Superlevels are averaged atomic energy levels with similar properties, and superlines are transitions between them. Details about different applications of this method to calculations of NLTE model atmospheres can be found in Dreizler and Werner (1993) and Hubeny and Lanz (1995). Since now the line blanketing in NLTE can be handled in a satisfactory manner and since there are also publicly available computer codes able to solve the problem, e.g. `TLUSTY`¹ (Hubeny, 1988; Hubeny and Lanz, 1995) or `PRO2`² (Werner and Dreizler, 1999; Werner et al, 2003), LTE line blanketed model atmospheres should be replaced by the NLTE ones.

The basic consequence of switching from LTE to NLTE is that differences in population numbers and also in ionization balance appear. The LTE populations and ionization fractions are systematically in error, especially in the outer parts of the atmosphere, which is the forming region of many spectral lines. The effect of correct treatment of the equations of kinetic equilibrium in NLTE model atmospheres is nicely illustrated in Figs. 5-9 of Lanz and Hubeny (2003). For Rosseland optical depths $\tau_R \lesssim 1$ the error of the ionization balance caused by the assumption of LTE is clearly seen. These errors directly influence the profiles of corresponding lines. In addition, they also influence heating and cooling in the stellar atmosphere and lead to differences in the temperature structure, as illustrated by the Figure 5 in Lanz and

¹ <http://nova.astro.umd.edu/index.html>

² part of TMAP, <http://astro.uni-tuebingen.de/~TMAP/>

Hubeny (2007). At large depths ($\tau_R \gg 1$), the radiation is close to isotropic and the diffusion approximation for radiation transfer can be used, which also means that the radiation is close to its equilibrium value. If also the particle velocities are close to the equilibrium distribution (as is common in “standard” stellar atmospheres), transition rates are very close to the detailed balance and the microscopic conditions for LTE are fulfilled there.

Since full treatment of NLTE model atmospheres may be computationally very time consuming, simplified method of solving the NLTE problem (radiative transfer + rate equations) for selected trace elements in a *given* model atmosphere is commonly being used. For more details about this approach we refer the reader to the book by Monier et al (2010). Unfortunately, using the LTE model atmospheres instead of the NLTE ones still dominates this approach. Besides the availability of the LTE models this is probably caused by the fact that the temperature structures of LTE and NLTE models are very similar at large depths. Some authors advocate using the hybrid method (LTE model atmosphere with NLTE radiative transfer for trace elements) to be equivalent to the full NLTE approach. Przybilla et al (2011) even concluded that “... *LTE and NLTE model atmospheres are essentially equivalent for dwarf and giant stars over the range $15000\text{ K} < T_{\text{eff}} < 35000\text{ K}$, for most practical applications*”, which can be true if practical applications are dealing only with lines forming at optical depths $\tau_R \gtrsim 1$. For lines forming above $\tau_R \approx 1$, which is the majority of spectral lines, we may expect differences.

Thus, full NLTE modeling (i.e. calculation of NLTE model atmospheres with the solution of the NLTE problem for trace elements) should be always preferred since it uses physically consistent assumptions (see Kubát, 2010). In this approach, the influence of radiation on level occupation numbers (hence opacities) is not neglected as in the LTE approach. To be sure that the results are correct, each particular application of the hybrid LTE/NLTE method has to be independently tested. We would like to emphasize that in any case, the hybrid LTE/NLTE approach is significantly superior to pure LTE analysis. To summarize, using LTE model atmospheres is a fast option, while using NLTE model atmospheres is a much more exact option, and should be preferred whenever possible. The best option to save computing time is to calculate NLTE model atmosphere as a background model, and then solve the NLTE problem for trace elements, if the conditions for using trace element approximation are fulfilled.

5 Model atom construction

An important part of the NLTE calculation is construction of a proper model of an atom or ion studied. Some ions are relatively simple, besides hydrogen it is also the neutral helium (e.g. Auer and Mihalas, 1972). On the other hand, the total number of levels and corresponding transitions may be enormous for some ions (see Fig. 5 of Hauschildt and Baron, 1995, where the number of transitions is too large to plot,

they form a continuous black surface and one can hardly find any relevant information from that figure).

To make the NLTE problem tractable, complicated model atoms may be simplified. It is usually done by assuming levels with high quantum number to be in LTE with respect to the ground level of the next ion. This way these levels do not enter the equations of statistical equilibrium. Another possibility is to merge levels, especially for multiplets (e.g. for neutral sodium, Gehren, 1975; Boyarchuk et al, 1988). The most sophisticated way to simplify model atoms is by creating superlevels, which can be applied to most complicated ions like iron and nickel. Superlevels are generalized multiplets, the energy levels of all levels from a superlevel are averaged (including proper statistical weights), and similarly the transitions to and from a superlevel members are averaged. Then the NLTE line formation problem is solved for model atom consisting of superlevels. An example how the superlevels can be created can be found in Hubeny and Lanz (1995).

Collecting data for all transitions is not an easy task for most of metallic ions. We have to collect ionization cross sections for all levels included, transition probabilities for all allowed or forbidden radiative transitions, and collisional cross sections for all possible transitions. If data are not available, we have to look for some reasonable approximation. Finally, we have to evaluate values for the merged levels, if they are used.

6 Hot stars with winds

Stellar wind is an outflow of matter from the stellar surface and it is a common property of hot massive stars. The strength of the wind depends on a spectral type, generally, higher stellar luminosity and lower stellar gravity support stronger stellar winds. This means that the strongest winds are for O-type supergiants while for dwarf A-type stars the winds are almost absent.

All O-type stars, including O-dwarfs, have stellar wind. Since these stars emit the maximum of their radiation in the UV wavelength region, the fact that they lose mass via stellar winds was discovered by analysis of first ultraviolet spectra of this stellar type (Morton, 1967) obtained by the *Aerobee* rocket. Observed spectra showed strong P-Cygni type line profiles, for such lines as of C IV and Si IV. For an example of P-Cygni type line profiles see in Fig. 1.

For hot massive stars, the mass-loss rates (dM/dt), which describe how quickly the star loses its mass, reach values up to $10^{-6} M_{\odot} \text{ year}^{-1}$. Terminal wind velocities grow from the photosphere and reach their maximum $v_{\infty} \sim 3000 \text{ km s}^{-1}$ far from the stellar surface. The outflow is driven by radiation, which is absorbed or scattered in continuum (by electrons and by bound-free and free-free transitions) and in spectral lines. The dominant contribution to radiative acceleration in these atmospheres comes from resonance ultraviolet lines of metals, where large flux in the ultraviolet part of spectrum meets large absorption in these lines, which is amplified by the Doppler shift caused by the velocity gradient. On the other hand, the

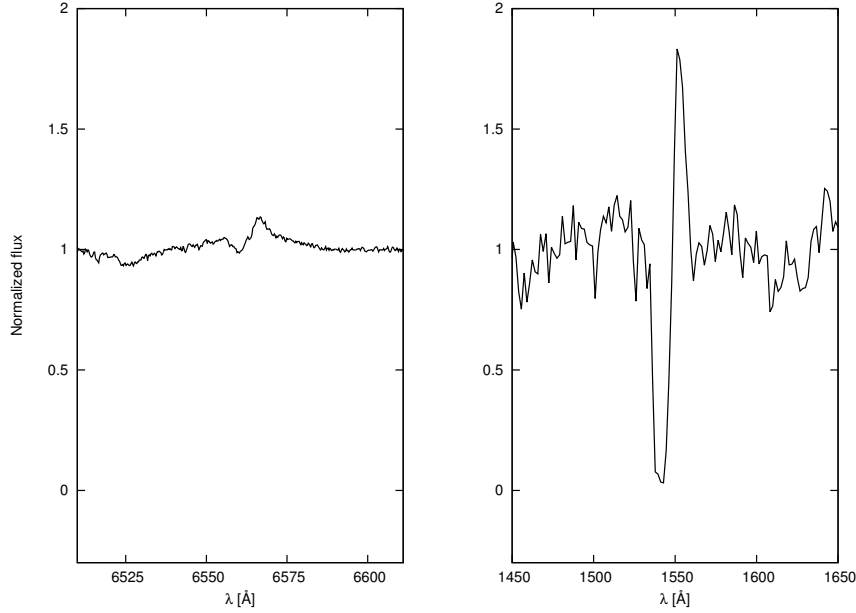


Fig. 1 Illustration of P-Cygni type profiles (normalised to continuum) of the line $H\alpha$ (left panel) and the ultraviolet line of C IV (right panel) for the star λ Cep. The ultraviolet spectrum is taken from the IUE archive (<http://archive.stsci.edu/iue/>), the visual spectrum was observed using the Ondřejov Perek Telescope.

most abundant elements, hydrogen and helium, gain negligible radiative force. The momentum gained by metals is transferred to hydrogen and helium by means of Coulomb collisions between charged ions of metals and hydrogen-helium component. Since winds are present practically in all O-type stars and supergiant B and A-type stars, they have to be taken into account in analysis of hot stars.

6.1 Modeling of hot stars with winds

The presence of an outflow is quite a complication in calculations of consistent models, which can predict theoretical spectra. To understand how radiation emerging from the stellar photosphere (static medium) changes passing through their expanding atmosphere, i.e. wind (moving medium), radiative transfer in both media has to be solved. There is a number of methods and computer codes for static media available, but they are not adequate to treat expanding atmospheres of hot stars. The problem of the transfer of radiation in moving media is more complicated, since the wind is expanding, and therefore the Doppler shift of the photon frequencies must be taken into account. Absorption and emission coefficients become angle depen-

dent. Consequently, these coefficients become anisotropic and the aberration of light may become important (the latter effect is usually neglected for stellar winds where $v/c \lesssim 0.01$, see Mihalas et al, 1976).

There are two basic classes of methods (see, e.g., Mihalas and Kunasz, 1986) for solving the radiative transfer equation in moving medium, namely the solution in the observer frame and the solution in the comoving frame. In the observer frame, the computations are straightforward, but the opacity and emissivity become angle dependent. Consequently, the number of frequency and angle points necessary to solve the radiative transfer equation may become enormous making the task computationally expensive. On the other hand, since the comoving frame is the local rest frame of the matter, opacity and emissivity are isotropic, but the expressions for solution of the radiative transfer are more complicated.

To simplify treatment of the problem, a *core-halo approximation* is commonly used, which means that photosphere and wind are modeled separately, and that the wind does not influence photosphere, while photospheric flux is a lower boundary condition for wind solution. Usually, the photosphere is assumed to be static and a full NLTE line-blanketed model atmosphere modeling described in the Section 3.1 is done. Here NLTE modeling is inevitable, since LTE is not valid in the photospheres of O stars. Then the photospheric flux is taken as a lower boundary condition for wind solution, which is usually performed for given velocity, density, and temperature structure, i.e. the NLTE line formation problem, solution of equations of statistical equilibrium together with the radiative transfer equation. Due to the large velocity gradients present in winds of these stars, Sobolev approximation may be used, and the radiative transfer is significantly simplified, since then the system of equations of statistical equilibrium and radiative transfer is local.

With this model, the analysis is done in steps. The lines which are expected not to be influenced by wind are selected (the photospheric lines). These lines serve for T_{eff} determination, similarly to static models. Then the wind line profiles are calculated for given velocity $v(r)$ and density $\rho(r)$ and the mass-loss rate is determined. Illustrative examples of application of such a procedure may be found in Bouret et al (2012). The most important computer codes for modeling of hot star winds are listed elsewhere in this book (Kubát, 2014). A more general background of the analysis of hot stars with winds may be found, e.g. in Puls et al (2008).

7 Summary

For hot stars NLTE analysis is necessary. It may be done using either LTE or better NLTE model atmospheres followed by NLTE for trace elements, if required. NLTE model atmospheres should be preferred, since they are more exact. The model atoms have to be carefully constructed. Model grids may save computing time. The systematic influence of stellar wind on emergent radiation has to be taken into account.

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